

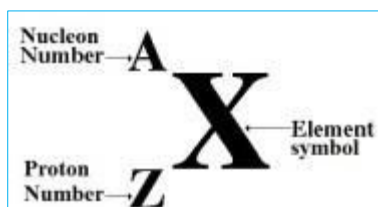


ATOMIC STRUCTURE

1. Particles in the atom and atomic radius

- Atoms consist of small, dense positively charged nucleus consisting of protons and neutrons, surrounded by negatively charged electrons

Particle	Relative charge	Mass (atomic mass units)
Proton	+1	1
Neutron	0	1
Electron	-1	1/1840



Proton number (atomic number) is the number of protons in the nucleus of an atom

Nucleon number (mass number) is the total number of protons and neutrons in the nucleus of an atom

- The mass of an atom is concentrated in the nucleus, because the nucleus contains the heaviest subatomic particles (the neutrons and protons)
- The electrostatic attraction between the positive nucleus and negatively charged electrons holds an atom together
- A beam of protons, neutrons and electrons moving at the same velocity in an electric field:
 - Protons – less and slow deflection towards negatively charged plate
 - Neutron – no deflection, go straight
 - Electrons – more and faster deflection towards positively charged plate

• Atomic radius (measure of the size of atoms)

- As we move from right to left of a periodic table, the atomic radii decrease as nuclear charge increases so electrons are pulled closer to the nuclei so the atom becomes smaller.
- As we move down a group, atomic radii increase as electrons are getting added up to new shells

• Ionic radius (measure of the size of ions)

- Increase with increasing negative charge – more electrons gained, weak force holding electrons and nuclei – larger ionic radii
- Decrease with increasing positive charge – electrons lost, more force, electrons pulled towards the nuclei – smaller ionic radii



2. Isotopes

- **Isotopes** are atoms of the same element that contain the same number of protons and electrons but a different number of neutrons
- The symbol for an isotope is the chemical symbol (or word) followed by a dash and then the mass number (eg. carbon-12 and carbon-14)
- Isotopes of the same element display the same chemical characteristics, as they have the same number of electrons in their outer shells
- Isotopes have different physical properties such as small differences in their mass and density

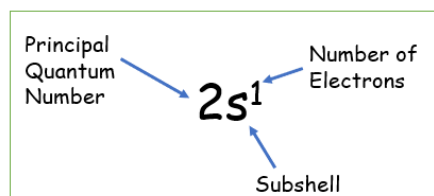
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3. Electrons, energy levels and atomic orbitals

- The arrangement of electrons in an atom is called the electronic configuration. Electrons are arranged around the nucleus in principal quantum shells

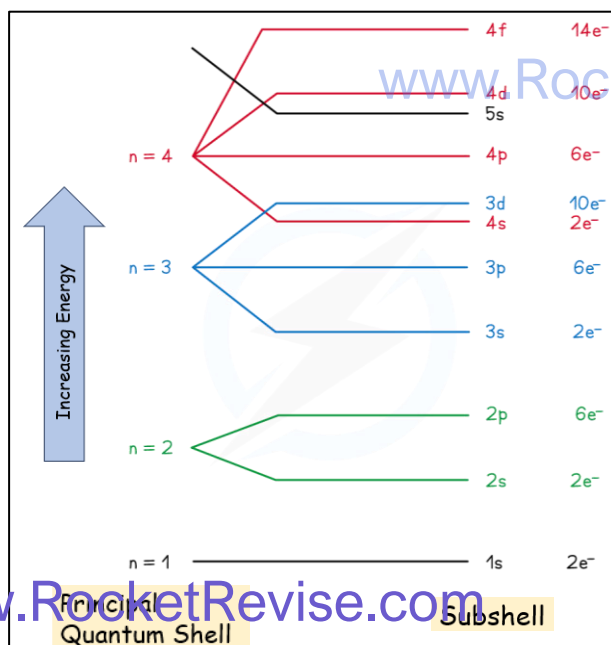
3.1 Principal quantum numbers (n)

- used to number the energy levels or quantum shells
- The higher the principal quantum number, the higher the energy of the shell, greater the distance it is from the nucleus
- Each principal quantum number has a fixed number of electrons it can hold
 - > n = 1: up to 2 electrons
 - > n = 2: up to 8 electrons
 - > n = 3: up to 18 electrons
 - > n = 4: up to 32 electrons



3.2 Subshells

- The principal quantum shells are split into subshells which are given the letters s, p and d
- The energy of the electrons in the subshells increases in the order $s < p < d$
- The order of subshells appears to overlap for the higher principal quantum shells as seen in the diagram below:





3.3 Orbitals

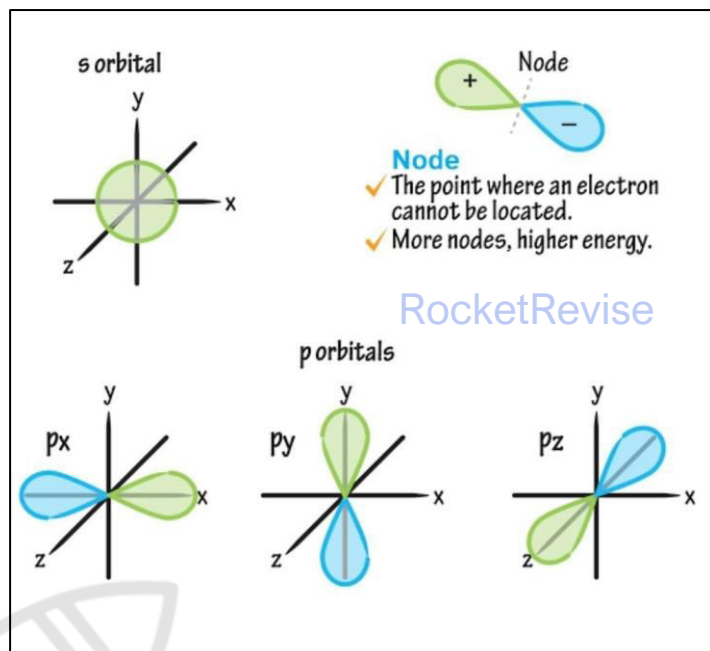
• Subshells contain one or more atomic orbitals. Each atomic orbital can be occupied by a maximum of two electrons

• This means that the number of orbitals in each subshell is as follows:

- s: one orbital ($1 \times 2 = 2$ electrons)
- p: three orbitals ($3 \times 2 = 6$ electrons)
- d: five orbitals ($5 \times 2 = 10$ electrons)
- f: seven orbitals ($7 \times 2 = 14$ electrons)

• Each subshell can hold a specific number of orbitals:

- s subshell: 1 orbital
- p subshell: 3 orbitals labelled p_x , p_y and p_z
- d subshell: 5 orbitals
- f subshell: 7 orbitals

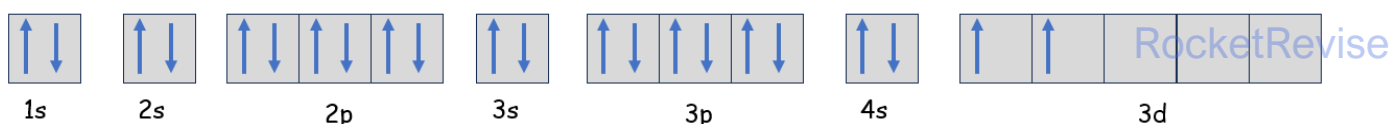


Principal Quantum Number, n (shell)	Subshells Possible (s, p, d, f)	Orbitals per subshell	Orbitals per principal quantum	Electrons per subshell	Electrons per shell
1	s	1	1	2	2
2	s	1	4	2	8
	p	3		6	
3	s	1	9	2	18
	p	3		6	
	d	5		10	
4	s	1	16	2	32
	p	3		6	
	d	5		10	
	f	7		14	



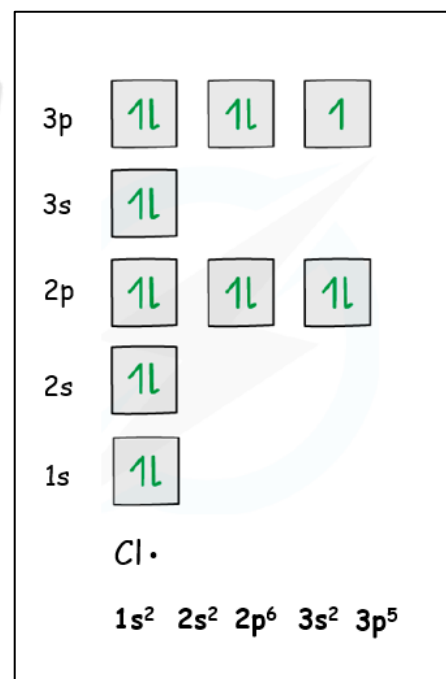
3.4 Electron Box Notation

- The electron configuration can also be represented using the electrons in boxes notation - each box represents an atomic orbital
- The boxes are arranged in order of increasing energy from lowest to highest
- The electrons are represented by opposite arrows to show the spin of the electrons
- The box notation for titanium (22) is shown below:



3.5 Free Radicals

- A free radical is a species with one or more unpaired electron
- The unpaired electron in the free radical is shown as a dot
 - Eg. a chlorine free radical has the electron configuration $1s^2 2s^2 2p^6 3s^2 3p^5$
 - Two of the three p orbitals have paired electrons whereas one of them has an unpaired electron



3.6 Example electronic configuration

- Potassium has 19 electrons, so the full electronic configuration is: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$
- Calcium has 20 electrons, so the full electronic configuration is: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$
- Abbreviated electron configuration of calcium is: (Ar) $4s^2$
- The 4s orbital is lower in energy than the 3d subshell and is therefore filled first
- Copper electronic configuration: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^1$ – because $3d^{10}$ is stable than $3d^9$ (exception) – expected configuration is: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^9$



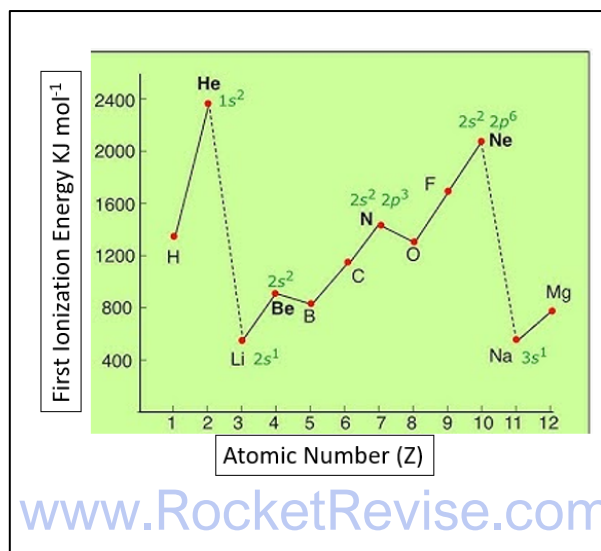
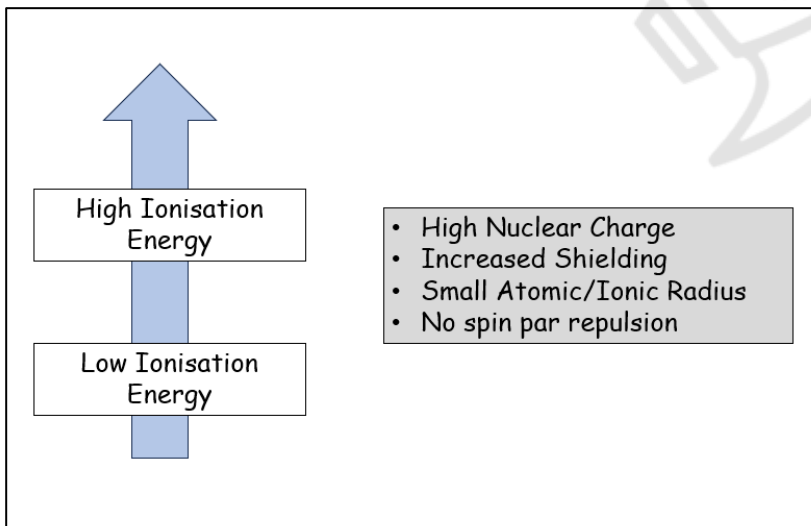
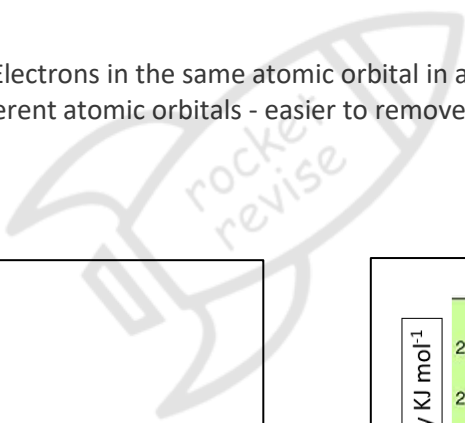
4. Ionisation energy

- Ionisation Energy (IE) of an element is the amount of energy required to remove one mole of electrons from one mole of gaseous atoms of an element to form one mole of gaseous ions

4.1 Factors affecting the size of ionization energy

- **Size of the nuclear charge:** The nuclear charge increases with increasing atomic number - higher attractive forces between the nucleus and electrons – higher ionisation energy
- **Distance of outer electrons from the nucleus:** Electrons in shells that are further away from the nucleus are less attracted to the nucleus - the nuclear attraction is weaker - lower the ionisation energy
- **Atomic radius:** lower the atomic radius, closer the shell is to the nucleus – higher attractive forces – higher ionization energy (ionization increases across a period from left to right)
- **Shielding effect of inner electrons:** the more shells an atom has, the greater the shielding effect (inner shells prevents outer shell to feel full nuclear charge) - lower the ionisation energy
- **Spin-pair repulsion:** Electrons in the same atomic orbital in a subshell repel each other than electrons in different atomic orbitals - easier to remove an electron – lower ionisation energy

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- The ionisation energy increases across a period and decreases down a group
- There will be a large increase in ionisation energy as it moves to the next shell



4.2 Ionisation energies: electronic configuration

Successive ionisation energy is the energy required to remove first, second, third..... electron

Can be used to:

- Predict or confirm the simple electronic configuration of elements
- Confirm the number of electrons in the outer shell of an element
- Deduce the Group an element belongs to in the Periodic Table

By analysing where the large jumps appear and the number of electrons removed when these large jumps occur, the **electron configuration** of an atom can be determined

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Sodium

- There is a huge increase in ionisation energy from the first to the second ionisation energy - easier to remove the first electron than the second
- the valence shell must contain only one electron indicating that sodium belongs to group I
- The large jump corresponds to moving from the 3s to the full 2p subshell →
Na $1s^2 2s^2 2p^6 3s^1$

Magnesium

- There is a huge increase in ionisation energy from the second to the third - easier to remove the first two electrons than the third
- the valence shell must contain only two electrons indicating that magnesium belongs to group II
- The large jump corresponds to moving from the 3s to the full 2p subshell →
Mg $1s^2 2s^2 2p^6 3s^2$

Aluminium

- There is a huge increase in ionisation energy from the third to the fourth - easier to remove the first three electrons than the fourth
- the valence shell must contain only three electrons indicating that aluminium belongs to group III
- The 3p electron and 3s electrons are relatively easy to remove as they have weakened shielding effects (far from nucleus)
- 2p electrons are harder to remove as it is located close to nucleus and experience greater nuclear charge
- The large jump corresponds to moving from the third shell to the second shell →
Al $1s^2 2s^2 2p^6 3s^2 3p^1$

Element	Atomic Number	First Ionization Energies KJ mol ⁻¹			
		First	Second	Third	Fourth
Na	11	494	4560	6940	9540
Mg	12	736	1450	7740	10500
Al	13	577	1820	2740	11600